XYZ

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xanthine

A purine base (2,6-diketopurine) that lies on the oxidative degradation pathway for purine nucleotides. It is derived from the oxidation of hypoxanthine and is subsequently further oxidized to urate (uric acid, 2,6,8-triketopurine). Both oxidations are catalyzed by the enzyme xanthine oxidase. Caffeine (1,3,5-trimethylxanthine) and theophylline (1,3-dimethylxanthine) are methylated derivatives of xanthine.

xanthine oxidase

A flavoprotein containing iron and molybdenum, xanthine oxidase [EC 1.1.3.22] that is capable of catalyzing two separate oxidations: one converting hypoxanthine to xanthine, the second producing urate (uric acid) from xanthine. Xanthine oxidase is a monooxygenase, incorporating one atom of oxygen from molecular oxygen (O_2) in hypoxanthine (or urate), while the other oxygen is transferred to water, forming hydrogen peroxide.

X-ray crystallography

One of two currently available methods to determine the structure of proteins and other large biomolecules. (The other method is multidimensional nuclear magnetic resonance, or NMR). The method of protein crystallography requires the purification, in milligram quantities, of the protein of interest, which is then subjected to conditions favoring the formation of crystals. With the proper degree of purity, homogeneity, and optimized crystallization conditions, the resulting protein crystals (usually less than a millimeter in dimension and around 50% in solvent content) will diffract a focused beam of X-rays.

The ordered arrangement of protein molecules in the crystalline lattice will produce a corresponding pattern in the measured diffraction intensities. The diffraction intensities, which are measured with image plates, multiwire detectors, or CCD cameras, are collected as completely as possible given the resolution limits of the data. These intensities relate to the underlying repeating motif of the crystal lattice - that is, the molecular structure of the protein, which is the goal of the method - but they are not sufficient for structure determination. Each measured point of diffraction has a phase, as well as an intensity, associated with it, and this phase information is not recoverable from the diffraction data of the native protein alone. This so-called phase problem is typically resolved by one of two tricks. One takes advantage of a pre-existing related structure. A set of initial phase estimates for the diffraction data of the unknown structure is taken from the expected diffraction data calculated from the known structure. This method is known as molecular replacement. The limitation of molecular replacement is the